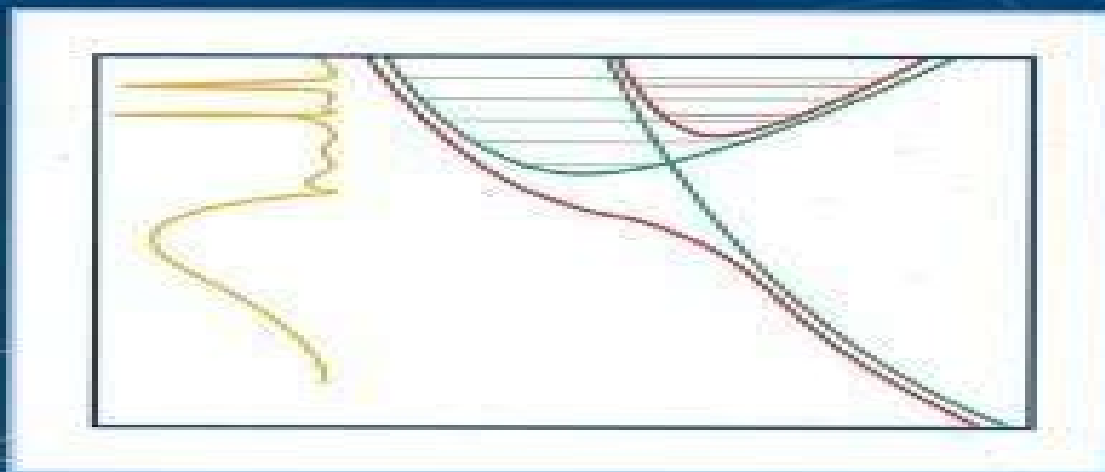


# The Spectra and Dynamics of Diatomic Molecules



Hélène Lefebvre-Brion  
and Robert W. Field

# Spectra And Dynamics Of Diatomic Molecules

**Jin-Ying Zhang**



## **Spectra And Dynamics Of Diatomic Molecules:**

*The Spectra and Dynamics of Diatomic Molecules* Helene Lefebvre-Brion, Robert W. Field, 2004-04-28 This book is written for graduate students just beginning research for theorists curious about what experimentalists actually can and do measure and for experimentalists bewildered by theory It is a guide for potential users of spectroscopic data and uses language and concepts that bridge the frequency and time domain spectroscopic communities Key topics concepts and techniques include the assignment of simple spectra basic experimental techniques definition of Born Oppenheimer and angular momentum basis sets and the associated spectroscopic energy level patterns Hund s cases construction of effective Hamiltonian matrices to represent both spectra and dynamics terms neglected in the Born Oppenheimer approximation situations intermediate between Hund s cases spectroscopic perturbations nonlinear least squares fitting calculation and interpretation of coupling terms semi classical WKB approximation transition intensities and interference effects direct photofragmentation dissociation and ionization and indirect photofragmentation predissociation and autoionization processes visualization of intramolecular dynamics quantum beats and wavepackets treatment of decaying quasi eigenstates using a complex Heff model and concluding with some examples of polyatomic molecule dynamics Students will discover that there is a fascinating world of cause and effect localized dynamics concealed beyond the reduction of spectra to archival molecular constants and the exact ab initio computation of molecular properties Professional spectroscopists kinetics ab initio theorists will appreciate the practical simplified model and rigorous theoretical approaches discussed in this book A fundamental reference for all spectra of small gas phase molecules It is the most up to date and comprehensive book on the electronic spectroscopy and dynamics of diatomic molecules The authors pioneered the development of many of the experimental methods concepts models and computational schemes described in this book

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*Advances in Chemical Physics, Volume 49* Ilya Prigogine, Stuart A. Rice, 2009-09-08 The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical authoritative evaluations of advances in every area of the discipline Filled with cutting edge research reported in a cohesive manner not found elsewhere in the literature each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics NASA Thesaurus ,1998 Contains the authorized subject terms by which the documents in the NASA STI Database are indexed and retrieved **State Selected and State-to-State Ion-Molecule Reaction Dynamics, Volume 82, Part 1** Cheuk-Yiu Ng, Michael Baer, 2009-09-09 State Selected and State to State Ion Molecules Reaction Dynamics details the recent experimental and theoretical accomplishments in the field to date by some of its foremost researchers and theorists Divided into two parts each of which separately describe the experimental and theoretical aspects of the field State Selected and State to State Ion Molecule Reaction Dynamics is an accessible well organized look at a highly useful and emerging chemical specialty Part 1 Experiment contains eight in depth studies which illustrate the key experimental work being done in the field today Chapter 1 provide a comprehensive review of the theory and application of inhomogeneous rf fields for the study of the dynamics of low energy ion molecules processes Chapter 2 describes the application of multiphoton ionization MPI for the preparation of reactant ion states Chapter 3 reviews the application of MPI schemes for state specific cross section measurements involving transition metal cations Chapter 4 describes the development of the threshold photoelectron secondary ion coincidence TESICO method Chapter 5 presents the conceptual and practical aspects of a multicoincidence technique Chapter 6 details the experimental results obtained using the photoionization and differential reactivity methods Chapter 7 reviews the several recent crossed beam studies of charge transfer and collision induced dissociation systems involving atomic and molecular ions Chapter 8 is a survey of 15 years of high resolution crossed beam scattering of protons with atoms diatoms and poly atomic molecules State Selected and State to State Ion Molecule Reaction Dynamics Part 1 Experiment offers professionals a true state of the science look at this fascinating and increasingly influential subject NBS Special Publication ,1978 *Microscopic to Macroscopic* Susan Kieffer, Alexandra Navrotsky, 2018-12-17 Volume 14 of Reviews in Mineralogy covers a short course about the relations among the microscopic structure of minerals and their macroscopic thermodynamic properties Understanding the micro to macro relations provides a rigorous theoretical foundation for formulation of energy relations With such a foundation measured parameters can be understood and extrapolation and prediction of thermodynamic properties beyond the range of measurement can be done with more confidence than if only empirical relations are used The purpose of this course is to consider the microscopic factors that influence the free energy of minerals atomic environments bonding and crystal structure These factors influence the structural energy and the detailed nature of the lattice vibrations which are an important source of entropy and enthalpy at temperatures greater than 0 K The same factors determine the relative energy

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